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Formation and Processing of Interstellar Dust

Grant NAG 5-938

(NASA-CR-194042) FORMATION AND PROCESSING OF INTERSTELLAR DUST Final Report (Union Coll.) 5 p

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David Peak
Principal Investigator
Professor of Physics
Union College
Schenectady, NY 12308
(518) 370-6342

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The work under grant NAG 5-938 consists of three main parts: theoretical studies of nucleation and growth kinetics, numerical simulations of small cluster properties, and experimental investigations of the mechanical characteristics of fluffy aggregates as laboratory analogs of condensed bodies in the early solar nebula.

Aided by this grant, my students and I have established a computational model to describe the nucleation and growth of refractory grains in stellar outflows. Our model integrates the kinetics equations which result when aggregation is pictured as a hierarchy of monomer-cluster interactions: a cluster of size j results from a cluster of size j-1 absorbing a monomer and/or from a cluster of size j+1 ejecting a monomer, and so on. Features which differentiate our model from ordinary aggregation kinetics studies include: a size dependent accomodation coefficient; different temperatures characterizing the carrier gas, the radiation field, and the internal degrees of freedom of each cluster; coupling of the reaction kinetics to the hydrodynamics of the wind; spatially varying temperatures and densities; an internally consistent treatment of the nucleation and the growth kinetics.

Because the kinetic coefficients change relatively slowly with cluster size for supercritical clusters, it is possible to scale the problem of integrating 10^8 equations (necessary if one is to describe the formation of clusters with linear dimension of about a micron) down to one in which only about 100 equations are needed. Nevertheless, the extraordinary stiffness of the resulting equations requires very tight numerical tolerances and fairly long computer run times (a few hours on a VAX 785 -- running in background) to produce a complete set of data, that is, concentrations of clusters of all sizes as functions of position out to 10 or so stellar radii. We have examined many different example situations to explore the qualitative behavior of our model.

Still to be done are some calibrating calculations for well-identified stellar parameters. We would also like to generalize our current model to account for the possibility of fractal cluster cross-sections and for cluster-cluster coalescence.

The aggregation kinetics calculations outlined above suggest that critical nuclei in stellar winds can often be extremely small, perhaps only two or three molecules in size. Unfortunately, the relevant properties of such very small clusters are not well-known. A promising method for determining reasonable values for the poorly known parameters is to exploit the results of molecular dynamics simulations. We have been writing and testing code to perform such simulations for the refractory materials of interest in grain formation. For realistic interaction potentials (short range, fairly deep, non-central) conservation of energy over many decades of interaction time is difficult to maintain. Consequently, we have been investigating the nuances of the simulation for much simpler potentials (deep Lennard-Jones potentials) to try to understand the detailed nature ofthe breakdown of the numerical procedures.

Our first attempts to understand the mechanical properties of fluffy, extremely low density powders concentrated on measuring the compressive response of such powder samples under static load. The primary powder studied was CAB-O-SIL, a commercially available fumed silica. While not a precise analog of primitive nebular condensate material, CAB-O-SIL does have an unusually low packing fraction (about 2%) -- similar, perhaps to what might be expected of the fractal-like aggregates postulated to exist during the earliest stages of condensation. In our studies we gently loaded the surface of our samples with a succession of dense plates and measured the resulting compression via x-ray absorption. All runs were conducted at vacuum to mitigate the effects of absorbed air. These measurements indicated an exponential relation between the resistive pressure exerted by the powder and the depth to which the load settled:

$$P(s) \propto \exp(2.2s),$$

where s is the compression depth (in cm). Despite our care to use loading plates with cross-section much smaller than the cross-section of our sample chamber we suspected that our data were still influenced by wall effects. Furthermore, we believed that it was possible that the mechanisms by which static forces were produced in the powder samples might be different from those responsible for frictional drag on a moving projectile -- the latter being much closer to what would have to be known in order to understand aggregate/aggregate collisions.

Consequently, we have revised our approach to this problem. We have built several new sample chambers which can be evacuated and in which projectiles of varying mass and cross-section can be dropped into powder samples of varying volume. Numerous runs have now been made of impacts of spherical projectiles in three powders of significantly different density (and packing fraction). Preparation of each powder sample consists of sifting into the vacuum chamber, then pumping on the sample for about three days while heating to drive off absorbed water. The crater left by the impacting projectile is profiled by the absorption of highly collimated x-ray (for CAB-O-SIL) or gamma-ray (for the other powders -- titanium dioxide and magnesium silicate) beams.

The results of the impacting experiments are summarized in Figure 1. The data show a remarkably universal behavior; the maximum crater depth depends on the square root of the kinetic energy of impact per unit cross-sectional area of the projectile irrespective of powder system, impact energy, or nature of the projectile. The constant of proportionality *does* depend on the powder impacted, with the primary determining factor the compressibility of that system.

That the data form universal families with total impact energy proportional to crater depth squared can be understood in terms of a simple model of the interaction of projectile and powder. In this picture, the projectile cleans out a fairly sharp crater (consistent with the observation that in the systems studied little compactification is seen transverse to the crater column), plowing a plug of displaced mass in front of it. The volume of this plug is proportional to the volume of the crater and grows linearly with crater depth, s. In some portion of the plug volume weak grain/grain bonds are broken and reformed leading to an effective frictional force of the form

$$F(s) = \mu A s$$

where μ characterizes the compressibility of the resisting powder as well as the intergrain bond strength and A is the cross-sectional area of the projectile. With these assumptions the equation of motion of the vertically falling, intruding projectile is

$$M\, dv/dt = Mg - F(s).$$

This equation is easily integrated leading to

$$MgH/A = \mu s^2/2$$

where H is the total (including prior to impact) vertical distance the projectile travels before coming to rest. This simple model is eminently consistent with the empirical data shown in Figure 1.

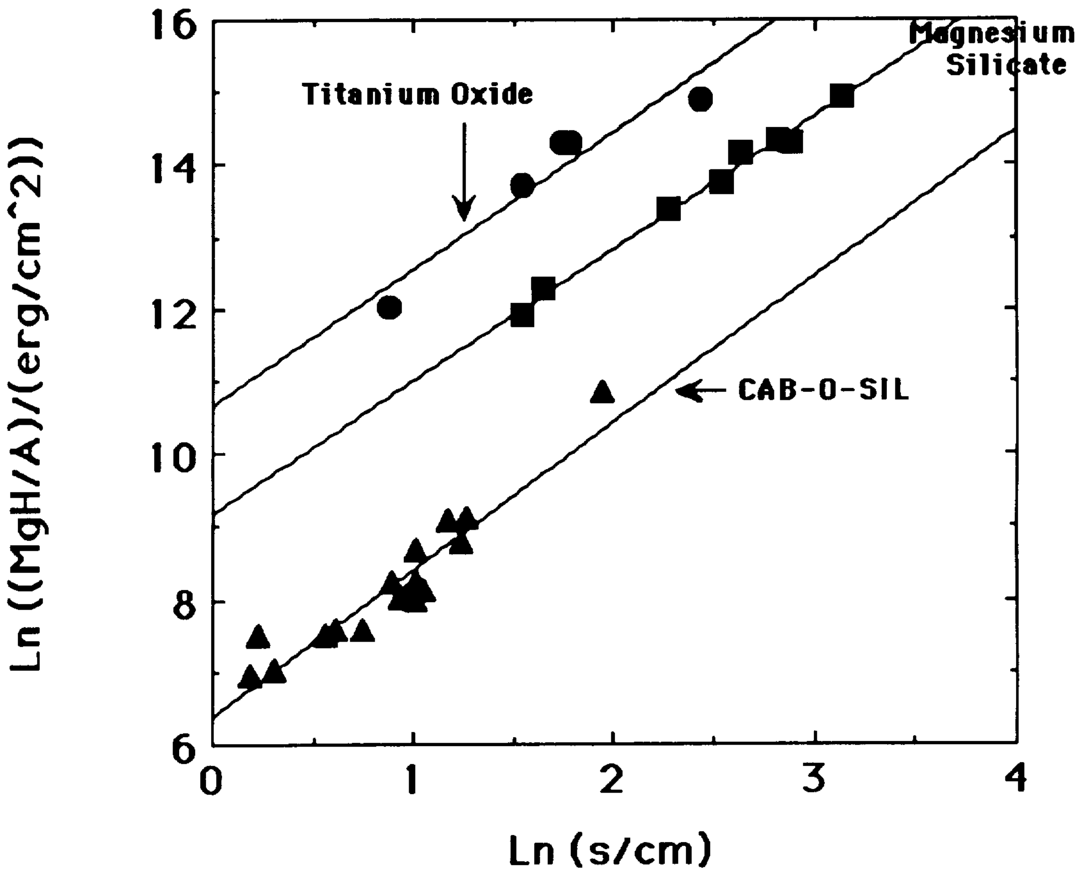

Figure 1.